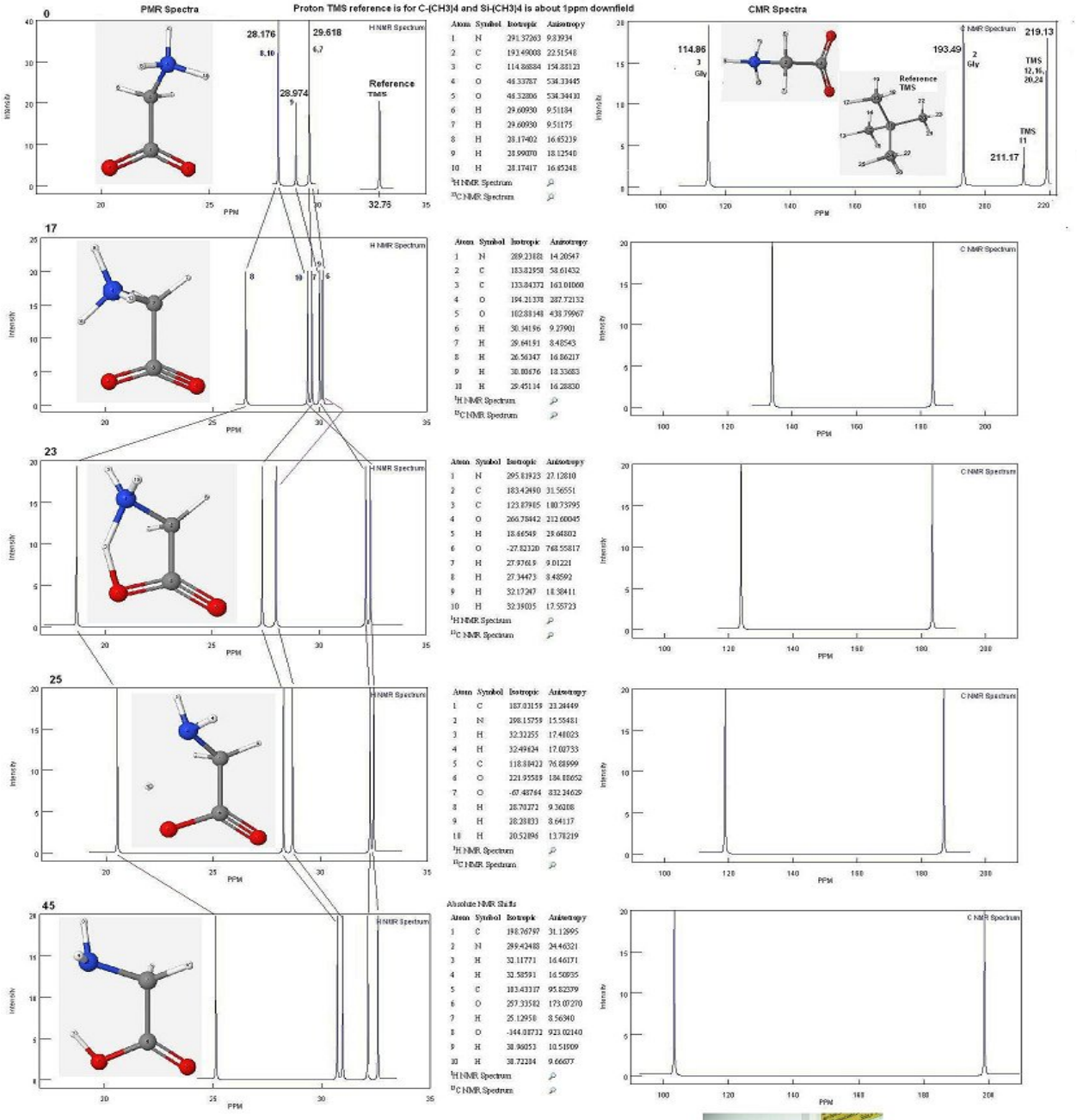


GLYCENE G.O. STRUCTURE SEQUENCE

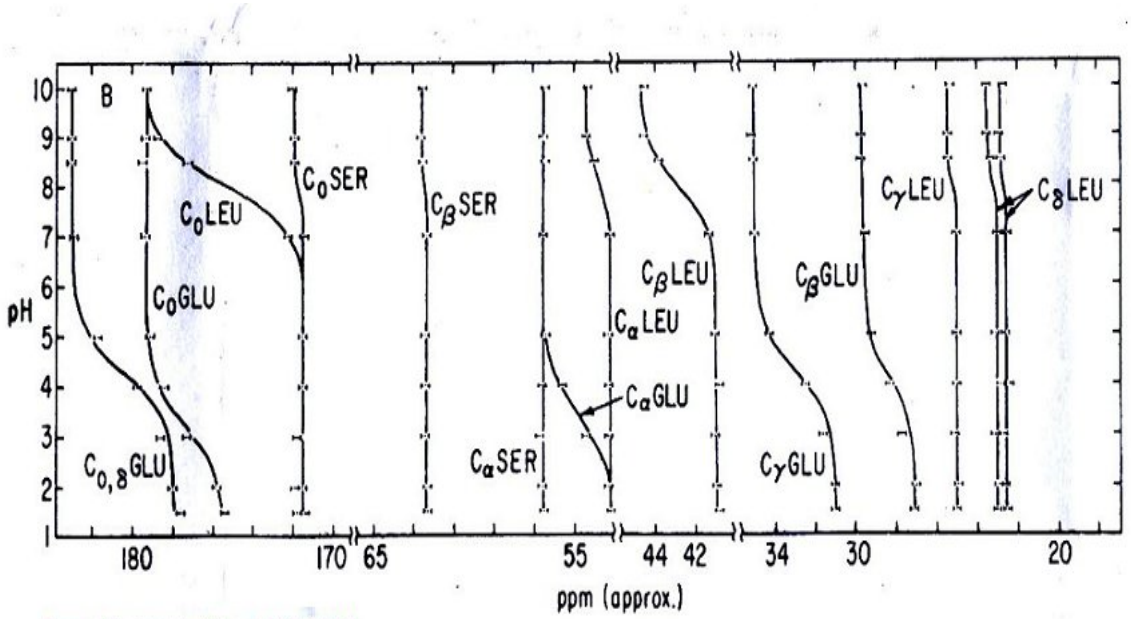
A few Selected Stages during the Optimization and the corresponding NMR Spectra with the View of the Molecule as inset

Input structure on top for iteration No.0 is Glycine Zwitterion. Iteration stages 17,23,25 & 45 are depicted above. At iteration 45 the result of G.O. is the nonionic form.

Aravamudhan

Theoretical Chemical Shift calculation and the Chemical shift spectra from the shift values is similar to the pH dependent shifts in the experimental Carbon NMR spectra in the next sheet

http://www.ugc-inno-nehu.com/crsi_13nsc_nmrs2007.html



From a Review article on 13C NMR

cited reference: J.Biol.Chem., Vol.246, p3725, (1971)

FIGURE 8.5.[21] *L-leucyl-L-seryl-L-glutamic acid dependence of cmr chemical shifts on pH.*

FOR Proton NMR all the protons in the alpha amino acids do not give prominently identifiable NMR lines. Thus conditions like solvent/pH etcetera have to be worked out to see the trends of variation with pH, and then to infer for the biological conditions

http://www.ugc-inno-nehu.com/crsi_13nsc_nmrs2007.html